Calculation of the cost matrix

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1 Problem statement and definitions

Let $y_{nj}$ be the data value at position (genomic coordinate) $n = 1, \ldots, N$ for replicate array $j = 1, \ldots, J$. Hence we have $J$ arrays and sequences of length $N$. The goal of this note is to describe an $O(NJ)$ algorithm to calculate the cost matrix of a piecewise linear model for the segmentation of the $(1, \ldots, N)$ axis. It is implemented in the function `costMatrix` in the package `tilingArray`. The cost matrix is the input for a dynamic programming algorithm that finds the optimal (least squares) segmentation.

The cost matrix $G_{km}$ is the sum of squared residuals for a segment from $m$ to $m + k - 1$ (i.e. including $m + k - 1$ but excluding $m + k$),

$$G_{km} := \sum_{j=1}^{J} \sum_{n=m}^{m+k-1} (y_{nj} - \hat{\mu}_{km})^2$$  (1)

where $1 \leq m \leq m + k - 1 \leq N$ and $\hat{\mu}_{km}$ is the mean of that segment,

$$\hat{\mu}_{km} = \frac{1}{Jk} \sum_{j=1}^{J} \sum_{n=m}^{m+k-1} y_{nj}.$$  (2)

Sidenote: a perhaps more straightforward definition of a cost matrix would be $G_{m'm} = G_{(m'−m)m}$, the sum of squared residuals for a segment from $m$ to $m' − 1$. I use version (1) because it makes it easier to use the condition of maximum segment length ($k \leq k_{\text{max}}$), which I need to get the algorithm from complexity $O(N^2)$ to $O(N)$. 


2 Algebra

\[ G_{km} = \sum_{j=1}^{J} \sum_{n=m}^{m+k-1} (y_{nj} - \hat{\mu}_{km})^2 \]  \hspace{1cm} (3)

\[ = \sum_{n,j} y_{nj}^2 - \frac{1}{Jk} \left( \sum_{n'j'} y_{n'j'} \right)^2 \]  \hspace{1cm} (4)

\[ = \sum_{n} q_{n} - \frac{1}{Jk} \left( \sum_{n'} r_{n'} \right)^2 \]  \hspace{1cm} (5)

with

\[ q_{n} := \sum_{j} y_{nj}^2 \]  \hspace{1cm} (6)

\[ r_{n} := \sum_{j} y_{nj} \]  \hspace{1cm} (7)

If \( y \) is an \( N \times J \) matrix, then the \( N \)-vectors \( q \) and \( r \) can be obtained by

\[ q = \text{rowSums}(y*y) \]
\[ r = \text{rowSums}(y) \]

Now define

\[ c_{\nu} = \sum_{n=1}^{\nu} r_{n} \]  \hspace{1cm} (8)

\[ d_{\nu} = \sum_{n=1}^{\nu} q_{n} \]  \hspace{1cm} (9)

which be obtained from

\[ c = \text{cumsum}(r) \]
\[ d = \text{cumsum}(q) \]

then (5) becomes

\[ (d_{m+k-1} - d_{m-1}) - \frac{1}{Jk} (c_{m+k-1} - c_{m-1})^2 \]  \hspace{1cm} (10)